Amendment to the Claims:

This listing of claims will replace all prior versions, and listing, of claims in the application.

Listing of Claims:

1. (currently amended) A computer implemented method of generating standardized representative three dimensional conformations of the molecular side chains derived from reactant molecules comprising the steps of:

a) defining a set of topomeric alignment rules; and

b) applying the topomeric alignment rules to the molecular side chains ~~reactants~~ to generate ~~the~~ a representative conformation~~s~~ for each.

2. (canceled)

3. (curently amended)A computer implemented method of characterizing the three dimensional structure of the molecular side chains derived from reactant molecules ~~reactants~~, which can assume many conformations, comprising the steps of:

a) generating standardized representative three dimensional conformations of the molecular side chains derived from reactant molecules comprising the steps of:

(1) defining a set of topomeric alignment rules; and

(2) applying the topomeric alignment rules to the molecular side chains ~~reactants~~ to generate ~~the~~ a representative conformation~~s~~ for each; and

b) ~~determining~~ generating the CoMFA steric fields for each aligned molecular side chain ~~reactant~~.

4. (previously presented) The method of claim 3 further comprising the addition of topomeric hydrogen bonding fields to the CoMFA steric fields.

5. (canceled)

6. (canceled)

7. (currently amended) A computer implemented method of applying a molecular structural descriptor to ~~a set of reactants~~ the molecular side chains derived from reactant molecules to determine similarity of shape comprising the following steps:

a) generating standardized representative three dimensional conformations of the molecular side chains derived from reactant molecules comprising the steps of:

(1) defining a set of topomeric alignment rules; and

(2) applying the topomeric alignment rules to the molecular side chains ~~reactants~~ to generate ~~the~~ a representative conformation~~s~~ for each; and

b) generating ~~determining~~ the CoMFA steric fields for each topomerically aligned molecular side chain ~~reactant~~; and

c) calculating the field differences between all pairs of molecular side chains ~~reactants~~

wherein smaller field differences reflect greater similarity of shape.

8. (previously presented) The method of claim 7 further comprising after step b the additional step of adding topomeric hydrogen bonding fields to the CoMFA fields.

9. (canceled)

10. (canceled)

11. (new) A computer implemented method for configuring the molecular side chains derived from reactant molecules into a standardized representative three dimensional conformation enabling comparison between the side chains of shape related properties, comprising the following steps:

a) defining topomeric alignment rules;

b) obtaining, or generating from two dimensional (2D) structural information, the three dimensional (3D) configuration of the molecular side chains represented by the three dimensional coordinates of the atoms comprising the side chains; and

c) repositioning the relative positions of the atoms in the side chains by adjusting torsions according to the topomeric alignment rules

wherein a standardized aligned topomeric conformation is produced for each molecular side chain.

12. (new) A computer implemented method of characterizing the three dimensional structure of the molecular side chains derived from reactant molecules, which can assume amy conformations, comprising the steps of:

a) configuring the molecular side chains derived from reactant molecules into a standardized representative three dimensional conformation comprising the steps of:

(1) defining topomeric alignment rules;

(2) obtaining, or generating from two dimensional (2D) structural

information, the three dimensional (3D) configuration of the molecular side chains represented by the three dimensional coordinates of the atoms comprising the side chains; and

(3) repositioning the relative positions of the atoms in the side chains by adjusting torsions according to the topomeric alignment rules; and

b) generating the CoMFA steric fields for each aligned molecular side chain.

13. (new) The method of claim 12 further comprising after step b the additional step of adding topomeric hydrogen bonding fields to the CoMFA fields.

14. (new) A computer implemented method of applying a molecular structural descriptor to ~~a set of reactants~~ the molecular side chains derived from reactant molecules to determine similarity of shape comprising the following steps:

a) configuring the molecular side chains derived from reactant molecules into a standardized representative three dimensional conformation comprising the steps of:

(1) defining topomeric alignment rules;

(2) obtaining, or generating from two dimensional (2D) structural information, the three dimensional (3D) configuration of the molecular side chains represented by the three dimensional coordinates of the atoms comprising the side chains; and

(3) repositioning the relative positions of the atoms in the side chains by adjusting torsions according to the topomeric alignment rules; and

b) generating the CoMFA steric fields for each topomerically aligned molecular side chain; and

c) calculating the field differences between all pairs of molecular side chains wherein smaller field differences reflect greater similarity of shape.

15. (new) The method of claim 14 further comprising after step b the additional step of adding topomeric hydrogen bonding fields to the CoMFA fields.